Propanamide, 2-hydroxy-2-methyl-13027-88-8 | DTXSID8065327

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 289 °C

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

Image not found

beta-Aminobutyric acid

Measured: 193 Predicted: 250 Image not found

Alanine, 2-methyl-Measured: 335 Predicted: 307